TSD-1c

Emissions Processing for 2002 OTC Regional and Urban 12km Base Year Simulation

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Overview

All emissions processing for the revised 2002 OTC regional and urban 12 km base case simulations was performed with SMOKE2.1 compiled on a Red Hat 9.0 Linux operating system with the Portland group fortran compiler version 5.1. The emissions processing was performed on a month-by-month and RPO-by-RPO basis, i.e. SMOKE processing was performed for each month for each of the RPOs (MANE-VU, VISTAS, CENRAP, MRPO) individually as well as for Canada. For each month/RPO combination, a separate SMOKE ASSIGNS file was created, and the length of the episode in each of these ASSIGNS files was set to the entire month. Also, as discussed in Section 3, there was no difference between "episode-average" temperatures and "monthly-average" temperatures for the Mobile6 simulations that used the option of temperature averaging.

This document is structured as follows: A listing of all emission inventories is given in Section 2, organized by RPO and source category. Section 3 discusses the Mobile6 processing approach employed for the different RPOs, while Section 4 describes the processing of biogenic emissions with BEIS3.12. Finally, Sections 5 through7 describe the temporal allocation, speciation, and spatial allocation of the emissions inventories, respectively.

1. Emission Inventories

1.1 MANE-VU

Version 3 of the MANE_VU inventory was utilized to generate CMAQ-ready emissions. This emissions inventory data were obtained from the MANEVU archive in April 2006.

1.1.1 Area Sources

- Files: MANEVU_AREA_SMOKE_INPUT_ANNUAL_SUMMERDAY_040606.txt and MANEVU_AREA_SMOKE_INPUT_ANNUAL_WINTERDAY_040606.txt prepared by PECHAN, downloaded from **ftp.marama.org** (username mane-vu, password exchange)
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing

1.1.2 Nonroad Sources

- File: MANEVU_NRD2002_SMOKE_030306 prepared by PECHAN; downloaded from **ftp.marama.org** (username mane-vu, password exchange)

1.1.3 Mobile Sources

- VMT/Speed: MANEVU_2002_mbinv_02022006_addCT.txt prepared by PECHAN and NESCAUM; downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

1.1.4 Point Sources

- Files: MANEVU_Point_SMOKE_INPUT_ANNUAL_SUMMERDAY_041006.txt and MANEVU_Point_SMOKE_INPUT_ANNUAL_WINTERDAY_041006.txt prepared by PECHAN were downloaded from **ftp.marama.org** (username mane-vu, password exchange)
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing
- Corrected the omission of 2,100 tons/year VOC emissions from several point sources in NJ. NJDEP provided updated IDA files on June 30 that were used for modeling.

1.2 CENRAP

The inventory data were obtained from the CENRAP ftp site in March 2006 and reflect version BaseB of the CENRAP inventory.

1.2.1 Area Sources

- Files:
    - CENRAP_AREA_SMOKE_INPUT_ANN_STATES_081705.txt
    - CENRAP_AREA_MISC_SMOKE_INPUT_ANN_STATE_071905.txt
    - CENRAP_AREA_BURNING_SMOKE_INPUT_ANN_TX_ NELI_071905.txt
    - CENRAP_AREA_MISC_SMOKE_INPUT_NH3_MONTH_{MMM} _072805.txt where {MMM} is JAN, FEB, … DEC
    - CENRAP_AREA_SMOKE_INPUT_NH3_MONTH_{MMM} _071905.txt where {MMM} is JAN, FEB, … DEC
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing
- Note about area and nonroad source SMOKE processing for the CENRAP region: All area source inventories (both annual and month-specific) were processed in

one step through SMOKE. SMK_AVEDAY_YN was set to N, so seasonal profiles were used to apportion the annual inventories numbers by month. This setting was also used for the nonroad processing performed in a separate step. This was necessary since the month-specific files had zero in their 'average-day' column and the annual total column reflects the "monthly emissions as annual totals" as per header line. Therefore, seasonal profiles are used to apportion both the annual and month-specific files. As described below, we utilized the temporal profiles and cross-reference files generated by CENRAP. However, we did not verify that this approach indeed leads to the intended monthly allocation of ammonia and nonroad emissions.

1.2.2 Nonroad Sources

- Files:
    - o CENRAP_NONROAD_SMOKE_INPUT_ANN_071305.txt
    - o CENRAP_NONROAD_SMOKE_INPUT_MONTH_{MMM}_071305.txt where {MMM} is JAN, FEB, … DEC

1.2.3 Mobile Sources

- VMT/Speed files:
    - o mbinv02_vmt_cenrap_ce.ida
    - o mbinv02_vmt_cenrap_no.ida
    - o mbinv02_vmt_cenrap_so.ida
    - o mbinv02_vmt_cenrap_we.ida

1.2.4 Point Sources

- File: CENRAP_POINT_SMOKE_INPUT_ANNUAL_DAILY_072505.txt
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

1.3 VISTAS

All VISTAS emission files were obtained from the Alpine Geophysics ftp site. They reflect version BaseG of the VISTAS inventory with the exception of fire emissions which reflect BaseF and BaseD. These files were downloaded between February and August, 2006.

1.3.1 Area Sources

- Files:

- o arinv_vistas_2002g_2453922_w_pmfac.txt
- o ida_ar_fire_2002_vistaonly_basef.ida
- Note: the header lines of these files indicate that the fugitive dust correction was already applied, so no further correction was performed.

1.3.2 Nonroad Sources

- Files:
  - o nrinv_vistas_2002g_2453908.txt
  - o marinv_vistas_2002g_2453972.txt

1.3.3 Mobile Sources

- VMT/Speed file: mbinv_vistas_02g_vmt_12jun06.txt

1.3.4 Point Sources

- Files:
  - o Annual:
    - egu_ptinv_vistas_2002typ_baseg_2453909.txt
    - negu_ptinv_vistas_2002typ_baseg_2453909.txt
    - ptinv_fires_{MM}_typ.vistas.ida where {MM} is 01, 02, 03, etc. depending on the month; these annual point fire files were generated as part of the VISTAS BaseD inventory and were obtained in January 2005
  - o Hour-specific:
    - pthour_2002typ_baseg_{MMM}_28jun2006.ems where {MMM} is jan, feb, mar, etc.
    - pthour_fires_{MM}_typ.vistas.ida where {MM} is 01, 02, 03, etc. depending on the month; these hourly point fire files were generated as part of the VISTAS BaseD inventory and were obtained in January 2005
- Note: No fugitive dust correction was performed for these files.

1.4 MRPO

MRPO emissions for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA to convert the MRPO BaseK inventory from NIF to IDA format. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) between April and June 2006.

1.4.1 Area Sources

- Files:
  - o Annual:
    - arinv_mar_mrpok_2002_27apr2006.txt
    - arinv_other_mrpok_2002_20jun2006.txt
  - o Month-specific:

- arinv_nh3_2002_mrpok_{mmm}_3may2006.txt where {mmm} is jan, feb, etc.
- dustinv_2002_mrpok_{mmm}_23may2006.txt where {mmm} is jan, feb, etc.

- Fugitive dust correction: This correction was performed only to the arinv_other_mrpok_2002_20jun2006.txt file using county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

- Note about area source SMOKE processing: SMOKE processing was performed separately for the annual and month-specific files. For the annual inventory processing, SMK_AVEDAY_YN was set to N, so seasonal profiles were used to apportion the annual inventories numbers by month. For the month-specific inventory processing, this variable was set to Y so that no seasonal profiles would be applied and the inventory numbers in the 'average day' column would be used. To save a SMOKE processing step, the annual "marine" inventory "arinv_mar_mrpok_2002_27apr2006.txt" was processed together with the annual "other area source" inventory "arinv_other_mrpok_2002_20jun2006.txt" even though it technically is part of the nonroad inventory.

1.4.2 Nonroad Sources

- Files: nrinv_2002_mrpok_{mmm}_3may2006.txt where {mmm} is jan, feb, etc.

1.4.3 Mobile Sources

- VMT/Speed file: mbinv_mrpo_02f_vmt_02may06.txt

1.4.4 Point Sources

- Files: ptinv_egu_negu_2002_mrpok_1may2006.txt
- Fugitive dust correction: This correction was performed only to the arinv_other_mrpok_2002_20jun2006.txt file using county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

1.5 Canada

1.5.1 <u>Area Sources</u>

- File: AS2000_SMOKEready.txt obtained from
  ftp://ftp.epa.gov/EmisInventory/canada_2000inventory
- Fugitive dust correction: We applied "divide-by-four" correction for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; this adjustment was performed outside SMOKE with in-house Fortran programs. No county/province-specific correction factors were available for Canada

1.5.2 <u>Nonroad Sources</u>

- File: NONROAD2000_SMOKEready.txt obtained from
  ftp://ftp.epa.gov/EmisInventory/canada_2000inventory

1.5.3 <u>Mobile Sources</u>

- File: MOBILE2000_SMOKEready.txt obtained from
  ftp://ftp.epa.gov/EmisInventory/canada_2000inventory
- Fugitive dust correction: applied "divide-by-four" correction for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; this adjustment was performed outside of SMOKE with in-house Fortran programs. No county/province-specific correction factors were available for Canada.

1.5.4 <u>Point Sources</u>

There has long been difficulty in obtaining an up-to-date Canadian criteria emissions inventory for point sources. This is due largely to confidentiality rights afforded to Canadian facilities. Thus far, the most recent inventory of Canadian point sources is rooted in the 1985 NAPAP data and is close to two decades old. Because there are a number of high emitting industrial facilities in southern Canada it is of particular importance to have a reasonably accurate inventory of these sources especially when modeling air quality over the Northeast and Midwest United States. Toward this end, an effort was made to obtain more recent Canadian point source data and incorporate it into an inventory database, which could then be used for the 2002 OTC air quality modeling.

Perhaps the most accurate and publicly accessible source of Canadian pollutant data is now available from the National Pollutant Release Inventory (NPRI) database. This database contains 268 substances. Facilities that manufacture, process or otherwise use one of these substances and that meet reporting thresholds are required to report these emissions to Environment Canada on an annual basis. The NPRI data are available at Environment Canada's website and can be found at the link http://www.ec.gc.ca/pdb/npri/npri_home_e.cfm. The page hosts an on-line search engine where one can locate emissions by pollutant or location. In addition, the entire database is available for download as an MS Access or Excel file. The NPRI database contains

numerous pages with a rather comprehensive list of information. Detailed information is available about each facility, including location, activity and annual emissions. In addition, facilities having stacks with a height of 50 meters or more are required to report stack parameters.

Unfortunately, one of the limitations of the NPRI database for modeling purposes is that the data are only available at the facility level. Emissions models require process level information, so in order to use this data, a few generalizations had to be made. Each facility has a Standard Industrial Classification (SIC) code associated with it; however, emissions models require Source Classification Codes (SCC's). SCC's are of critical importance as the emissions models use these codes for assignment of temporal and speciation profiles. SIC codes describe the general activity of a facility while SCC codes describe specific processes taking place at each facility. While no direct relationship exists between these two codes, a general albeit subjective association can be made.

For the purposes of creating a model-ready inventory file it was necessary to obtain the whole NPRI database. After merging all the necessary components from the NPRI database required in the SMOKE inventory file, the SIC code from each facility was examined and assigned an SCC code. In most cases, only a SCC3 level code was assigned with confidence. While this is admittedly a less than desirable process, it does allow for the use of the most recent emissions from the NPRI database to be used in modeling. Furthermore, having some level of SCC associated with these emissions will ensure that they will be assigned a temporal and speciation profile by the model, other than the default. Once the model-ready inventory file was developed, it was processed through SMOKE.

2. Mobile6 Processing

2.1 MANE-VU

2.1.1 Mobile6 input files

- Month-specific input files were prepared by PECHAN and NESCAUM and were downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar
- Added the line "REBUILD EFFECTS   :0.10" to each file before the SCENARIO record to override the Mobile6 default setting of 0.9 (90%) for the "chip reflash" effectiveness

2.1.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files were prepared by PECHAN and NESCAUM and were downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

2.1.3 <u>Temperature averaging</u>

- Following the setting in the MANEVU_2002_mvref.txt files, the following procedures were used by SMOKE for temporal and spatial temperature averaging in the calculation of emission factors:
    o Spatial averaging: temperatures were averaged over all counties that share a common reference county (i.e. Mobile6 input file)
    o Temporal averaging for May – September emissions processing: no temporal averaging was used, i.e. day-specific temperatures were used to calculate emission factors for each day.
    o Temporal averaging for non-summer-months emissions processing: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.2 CENRAP

2.2.1 <u>Mobile6 input files</u>

- Mobile6 input files for the CENRAP region for January and July were contained in the files central_M6_{MMM}.zip, north_M6_{MMM}.zip, south_M6_{MMM}.zip, west_M6_{MMM}.zip where {MMM} is either jan or jul. July input files were used for April – September processing, while January input files were used for the remaining months
- All files were downloaded from the CENRAP ftp site in March 2006.

2.2.2 <u>SMOKE/Mobile6 auxiliary files</u>

- SMOKE/Mobile6 auxiliary files were contained in the files central_M6_RD.zip, north_M6_RD.zip, south_M6_RD.zip, and west_M6_RD.zip. The SMOKE MCREF, MVREF, and MCODES files were contained in the file MOBILESMOKE_Inputs.zip. The MCREF and MVREF files were combined for the different regions ("central", "east", "west", "north")
- All files were downloaded from the CENRAP ftp site in March 2006.

2.2.3 <u>Temperature averaging</u>

- The following procedures were used by SMOKE for temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvref files:
    o Spatial averaging: no spatial averaging of temperatures, i.e. the temperatures for the reference county is used to calculate emission factors for all counties that share this reference county (i.e. Mobile6 input file)
    o Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.3 VISTAS

2.3.1 Mobile6 input files

- Month-specific Mobile6 input files were obtained from the Alpine Geophysics ftp site in July 2006. They reflect version BaseG of the VISTAS inventory.

2.3.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files utilized were obtained from the Alpine Geophysics ftp site in July 2006. They reflect version BaseG of the VISTAS inventory.

2.3.3 Temperature averaging

- The following procedures were used by SMOKE for the temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvref_baseg.36k.ag.txt file:
  - Spatial averaging: temperatures averaged over all counties that share a common reference county (i.e. Mobile6 input file)
  - Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.4 MRPO

2.4.1 Mobile6 input files

- Month-specific Mobile6 input files for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA. They are based on version BaseK of the MRPO inventory. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) in May 2006.

2.4.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA. They are based on version BaseK of the MRPO inventory. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) in May 2006.

2.4.3 Temperature averaging

- The following procedures were used by SMOKE for the temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvreg_mrpo_basek.txt file:
  - Spatial averaging: temperatures averaged over all counties that share a common reference county (i.e. Mobile6 input file)

o Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

3. Biogenic Emission Processing

Hourly gridded biogenic emissions for the 12 km and 36 km modeling domains were calculated by BEIS3.12 through SMOKE, using MCIP-processed MM5 fields for temperature ("TA", layer-1 temperature), solar radiation ("RGRND"), surface pressure ("PRES"), and precipitation ("RN" and "RC"). A 'seasonal switch' file was generated by the SMOKE utility metscan to determine whether winter or summer emission factors should be used for any given grid cell on any given day. Winter emission factors are used from January 1st through the date of the last frost and again from the data of the first frost in fall through December 31st. Summer emission factors are used for the time period in between. This calculation is performed separately for each grid cell.

4. Temporal Allocation

4.1 MANE-VU

4.1.1 Area and nonroad sources

- Generated as part of the MANE-VU version 1 inventory
- amptpro.m3.us+can.manevu.030205.txt
- amptref.m3.manevu.012405.txt
- downloaded from **ftp.marama.org** (username mane-vu, password exchange) in January 2005

4.1.2 Mobile sources

- MANEVU_2002_mtpro_02022006_addCT.txt
- MANEVU_2002_mtref_02022006_addCT.txt
- prepared by PECHAN and NESCAUM and downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

4.1.3 Point Sources

- Based on the same files as for the MANE-VU area and nonroad temporal files listed above, but added the CEM-based 2002 state-specific temporal profiles and cross-references for EGU sources for the MANE-VU states that were generated by VISTAS for their BaseD modeling and obtained in February 2005.
- No CEM-based hour-specific EGU emissions were utilized

4.2 CENRAP

The following temporal profiles and cross-reference files were used:

- Area and nonroad sources:
    - amptpro.m3.us+can.cenrap.010605_incl_nrd.txt
    - amptref.m3.cenrap.010605_add_nh3_and_nrd.txt
- Mobile sources:
    - mtpro.cenrap.v3.txt
    - mtref.cenrap.v3.txt
- Point sources:
    - ptpro.{QQ}.cenrap_egus_cem.00-03avg.121205.txt where {QQ} is Q1 for January/February/March, Q2 for April/May/June, etc.
    - ptref.{QQ}.cenrap_egus_cem.00-03avg.121205.txt where {QQ} is Q1 for January/February/March, Q2 for April/May/June, etc.
- All files were downloaded from the CENRAP ftp site in March 2006.

4.3 VISTAS

The following month-specific temporal profiles and cross-reference files were used:
- Area and nonroad sources:
    - atpro_vistas_basef_15jul05.txt
    - atref_vistas_basef_15jul05.txt
- Mobile sources:
    - mtpro_vistas_basef_04jul05.txt
    - mtref_us_can_vistas_basef_04jul05.txt
- Point sources:
    - ptpro_typ_{MMM}_vistasg_28jun2006.txt where {MMM} is jan, feb, mar, etc.
    - ptref_typ_vistas_baseg_28jun2006.txt
- These files were obtained from the Alpine Geophysics ftp site. They reflect version BaseG of the VISTAS inventory for the point source allocation files and version BaseF for the area, nonroad, and mobile source allocation files. These files were downloaded between February and July, 2006.

4.4 MRPO

The following month-specific temporal profiles and cross-reference files were used for all source categories:
- amptpro_typ_us_can_{MMM}_vistas_27nov04.txt where {MMM} is jan, feb, mar, etc.
- amptref_2002_us_can_vistas_17dec04.txt
- These files were obtained from VISTAS in January 2005 and reflect their BaseD modeling. No updated temporal profiles or cross-reference files were developed for use with the MRPO BaseK inventory.

4.5 Canada

For Canada, the SMOKE2.1 default temporal profiles and cross-reference files (amptpro.m3.us+can.txt and amptref.m3.us+can.txt) were utilized.

5. Speciation

The same speciation profiles (gspro.cmaq.cb4p25.txt) and cross-references (gsref.cmaq.cb4p25.txt) were utilized for all regions and all source categories. Different versions of these files were obtained (SMOKE2.1 default, EPA-CAIR modeling, VISTAS, CENRAP and MANE-VU) and compared. After comparing the creation dates and header lines of these files, it was determined that the EPA-CAIR and MANE-VU files had the most recent updates, and consequently the final speciation profile and cross-reference files used for all regions and source categories was based on the EPA-CAIR files with the addition of MANE-VU specific updates.

6. Spatial Allocation

6.1 U.S.

The spatial surrogates for the 12km domain were extracted from the national grid 12km U.S. gridding surrogates posted at EPA's website at
http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html
The gridding cross-references were also obtained from this website, but for the processing of MANE-VU area source emissions, MANE-VU specific cross-reference entries posted on the MARAMA ftp site were added.

6.2 Canada

The spatial surrogates for Canadian emissions for the 12km domain were extracted from the national grid 12km Canadian gridding surrogates posted at EPA's website at
http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html
The gridding cross-references were also obtained from this website.

Reference:

Pechan: (2006) Technical Support document for 2002 MANE-VU SIP Modeling inventories, version 3. Prepared by E. H. Pechan & Associates, Inc. 3622 Lyckan Parkway, Suite 2005, Durham, NC 27707.